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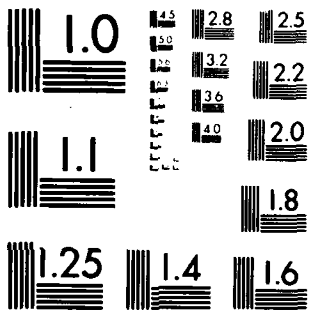


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THEORETICAL STUDIES OF THE INTERACTION OF RADIATION WITH MATTER

FINAL REPORT

STEVEN T. MANSON

FEBRUARY 29, 1980



U. S. ARMY RESEARCH OFFICE

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Work on the interaction of radiation with matter is described. In particular photoabsorption by ions and excited states is discussed, along with positive ion properties Born approximation results for EDST charged particle impact ionization of atoms. The relevance of these areas to various applied areas such as radiation protection and safety, x-ray laser schemes and effects, nuclear pumped lasers, and IR detection is pointed out.

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Over the period of these grants from the U.S. Army Research Office, we have been actively engaged in research into theoretical atomic and ionic physics. In what follows the major areas of our investigations shall be discussed, along with the progress that has been made in those areas. In addition, we shall also discuss, where applicable, the relevance of the research findings to various Army needs in the area. The discussions are as non-technical as possible, but ample references are given to published works where the technical details can be found.

## I. Photoabsorption by Positive Ions

Data on positive ion photoabsorption is required in modeling the effects of atmospheric thermonuclear blast. This knowledge is required not only to gain some insight into the vulnerability of missiles and other weapons,[1] as well as to understand the limitations that such a blast puts on radar.[2] In the blast, tremendous amounts of electromagnetic radiation (photons) are produced and issue forth through the atmosphere. The very high temperature of the blast creates an environment in which essentially all of the atmospheric gases are ionized. Thus an understanding of the transport of this electromagnetic energy from the site of the blast requires a knowledge of the cross sections for photoabsorption by positive ions.

In addition, with the possibility of an x-ray laser, one needs to know about the passage of x-rays through the atmosphere, as well as through various materials, to gain some insight into the amount delivered to the target. Since the x-rays rapidly ionize everything in their path, the problem is essentially one of photoabsorption by positive ions.[3]

It is important to note that it is extremely difficult to measure ionic photoabsorption in the laboratory owing to the extremely high temperatures required to produce them in quantity. Thus theoretical work is a necessity.

When we first began this work, our computer code, which had been written for atomic photoabsorption[4] was redesigned to do ions. Detailed studies of oxygen[5,6] and iron[7] were performed and some substantial simplifications for inner shell photoabsorption were uncovered; in particular we found that, apart from a shift in threshold, inner shell photoabsorption is almost completely unaffected (less than 3%) by the removal of outer shell electrons. This fact both allowed the transfer of extensive experimental experience on the neutrals to ions, as well as substantially reduced the work involved in the calculations.

We have also compared the accuracy of our results to highly sophisticated calculations[8] and can now predict, a priori, the few regions where the calculations are likely to be in errors by more than 10-20%. The two recent experiments[9,10] on $Li^+$ and $Na^+$, moreover, have shown excellent agreement with our calculations.

Thus, using our experience, we have produced a compendium of photoabsorption cross sections for atoms and ions for all of the elements from He(Z = 2) to Zn(Z = 30)[11]. In addition, our computer code itself has been adapted to BRL needs and is now part of their program library and an integral part of the nuclear fireball code.[1,12] The work has since been extended to include relativistic effects and heavy ions and we find that our conclusions concerning inner shells are unaffected.

even for 80 times ionized Th(Z = 90).[12] We, therefore, conclude this section by noting that owing to this work, we now have a rather thorough understanding of the physics as well as the quantitative aspects of photoabsorption by positive ions over the entire periodic table.

## II. Properties of Positive Atomic Ions

As discussed in Sec. I, highly stripped atomic ions are produced in large quantities in various situations of interest for defense applications, with very little possibility for determining their properties in the laboratory. Thus a project has been launched to study their properties theoretically. The chief result of our investigations, aside from a massive base of ionic data, is that there are alternative ways of mapping ionic properties.[13,14] Any ionic property can be regarded as a function of two variable, nuclear charge, Z, and electron number, N. Thus ionic data can be analyzed in terms of at least three pictures: isoelectronic (constant N), isonuclear (constant Z), and isoionic (constant $z = Z - N$). The three pictures are mutually complementary; they emphasize differing aspects of the systematics of ionic data as a function of Z and N. The isoelectronic picture has a long history; the other two were suggested by us[13,14] and recently have seen an upsurge in use.

The isoelectronic picture is the most straightforward and simple from a computational point of view. In addition, it is directly applicable to 1/Z expansion theory. All ionic properties approach known hydrogenic values, when plotted vs. 1/Z, in the limit $1/Z \to 0$ $(Z \to \infty)$. The isonuclear picture simplifies the variation of certain ionic properties from one order of the spectrum to the next. In particular, it spotlights the sensitivity of ionic properties to removal of electrons. Thus the isonuclear picture is well suited to certain applications such as the impurity contamination in CTR plasma; the many ions of a given impurity nuclide form an isonuclear sequence. These considerations are relevant to weapons applications as well. The isoionic picture maintains a constant asymptotic potential, $(z+1)/r$, in the ion. It thus focusses on the interplay between increasing Z and N simultaneously. Since the neutral atoms form the $z = 0$ isoionic sequence ($Z = N$), the use of this picture provides a framework for the transfer of extensive experience with the neutral atomic periodic system acquired through spectroscopy and collision physics.

The systematics of any ionic property could be studied in any one of the above pictures. Since, however, each picture emphasizes differing aspects of the variation of ionic properties, one picture will generally be most instructive for a given property. It is often not clear *a priori* which picture this will be in a particular situation so that each picture should be tried. We have emphasized this point, particularly to those who generate experimental or theoretical data on ionic properties, and urge that the data be looked at in the different pictures to glean the maximum amount of information.

In our own work, from the isonuclear picture we have learned that all inner shell ionic properties are virtually unaffected by removal of outer shell electrons[13,14] which allows us to use the extensive neutral data for ions. From the isoionic picture we have understood that the rich variation of structure associated with chemical properties of the neutral atoms, lessens considerably for the singly ionized, and is absent for higher stages of ionization.[13,14]

## III. Photoabsorption by Excited Atoms

Excited states of atoms are also produced in any very hot environment, such as those discussed in the previous sections; thus their properties are of interest. In addition, a possible detector in the IR range, with a quantum efficiency of unity, is now theoretically possible using lasers to excite atoms to states whose ionization potentials are in the IR range. Thus photoabsorption cross section for excited atomic states are needed.

In our preliminary studies, we have emphasized the alkali atoms whose ionization potentials are low enough to make them easily amenable to excitation via laser. One particularly interesting result was that several extra minima, including one dramatic minimum, appear in the cross section for Cs 5d photoabsorption.[15] These minima do not appear in the ground states of any atoms and are entirely a function of the diffuseness of the excited state wave function. Nor are these minima isolated phenomena - they span a broad range of states and elements.[16] We are now in the process of doing extensive work on all of the alkali atoms.

On a related matter, we have performed calculations on the ionization of metastable He $2^{1,3}s$ atoms by electron impact.[17] These calculations, done within the framework of Born approximation, have been rather successful in reproducing experimental results, and, as such, offer a strong possibility of being accurately predictive for a number of cases not amenable to laboratory study.

## IV. Charged Particle Impact Ionization of Atoms

The range and energy loss of charged particles passing through matter is almost solely related to the energy loss via ionization of the matter by the charged particles. Thus a knowledge of these cross section is the main constituent of calculations of radiation protection and shielding of both men and materials.

Another important application is for the possibility of nuclear-pumped lasers, i.e., dealing with the energy transfer of energetic fission fragments to a (hopefully) lasing medium. Ionization cross sections of the medium materials, along with the spectrum of secondary electrons which cause further ionizations and excitations, are of crucial importance in modelling the nuclear-pumped laser situation.[18]

In still another situation, that of the passage of an ion beam through the atmosphere or other media, the limiting factor of its penetration is the cross section for inelastic collisions, which are mostly ionization.

Finally, ionization cross sections of atoms by charged particle impact is of importance in the possibility of creating population inversions which are useful in deducing possible schemes for an x-ray laser. Thus these cross sections, which are of interest for all three of the above applications, are needed. Many of them are either unobtainable experimentally (at the present level of technology) or simply unavailable. Thus, the need for theoretical estimates is great.

Our work has dealt with total cross sections, single differential cross section (SDCS) or energy distribution of secondary electrons, and double differential cross sections (DDCS) or energy and angular distribution of secondary electrons. The total and SDCS are the primary results needed as input for the applied areas, but the SDCS is necessary to elucidate ionization mechanisms and to fully assess the validity of the calculational work.

The noble gases have been dealt with primarily owing to the fact that most of the experimental data extant is for the noble gases. The calculations were carried out within the framework of Born approximation which has proved to be far better than was hitherto suspected. Detailed calculations of the DDCS for electron and proton impact ionization of helium and argon[19,21] have shown excellent agreement with experiment in most energy and angular ranges. In addition, we have confirmed that the process of charge transfer to the continuum is responsible for the forward peaking at small angles. These calculations have been carried out for proton energies from 0.1 - 10 MeV, a factor of 100 in energy, and as a result, we have an excellent <u>predictive</u> prescription for obtaining DDCS for atoms and energies which cannot, as yet, be studied in a laboratory environment.

We have also studied the SDCS for a number of cases.[22,23] The focus of this work was to provide a predictive calculational scheme, as above, as well as to provide a check on experimental consistency and accuracy. In this latter realm, it has been noted for electron impact[24,25] that the ratio of the SDCS to the corresponding Rutherford cross section takes on a particularly simple form, being proportional to the optical (photoionization) cross section for small energy transfer, and is equal to the number of target electrons participating in the collision for large. We have extended this analysis to proton impact data recently. The importance of this analysis is that we can transfer a large body of optical data to charged particle collisions and we are now able to provide the SDCS for many targets in a simple way to an accuracy of ±30% (which is good enough for most modelling applications) doing virtually no calculations at all! Work is continuing in the direction of extrapolating existing experimental data with regard to incident energy and secondary electron energy.

We have further studied an interesting effect in the total ionization cross section for certain atomic subshells where a shoulder is seen on the low energy side of the maximum.[26] This effect was explained in terms of the fundamental quantity governing the ionization process, the generalized oscillator strength.[27] It was also pointed out how ubiquitous the phenomenon is, and the circumstances under which it can be found.

## References


1. J. Lacertera, G.R. Daum, and G.J. Klem, The BRL Nonequilibrium Nuclear Fireball Code: Thunderball, BRL Rpt. No. 1992, June, 1977.
2. J. Lacertera and G.R. Daum, Effects on Nonequilibrium Phenomena on Radar Transmission - Nonequilibrium Ionization, Tech. Rept. ARBRL-TR-02058, May 1978.
3. H. Jones, BRL (Private communication).
4. S.T. Manson and J.W. Cooper, Phys. Rev. 165, 126 (1968).
5. D.W. Missavage and S.T. Manson, Phys. Lett. A.
6. D.W. Missavage, S.T. Manson, and G.R. Daum, Phys. Rev. A 15, 1001 (1977).
7. R.F. Reilman and S.T. Manson, Phys. Rev. A 18, 2124 (1978).
8. A. Msezane, R.F. Reilman, S.T. Manson, J.R. Swanson, and L. Armstrong, Jr., Phys. Rev. A 15, 668 (1977).
9. T.B. Lucatorto and T.J. McIlrath, Phys. Rev. Lett. 37, 428 (1976).
10. T.J. McIlrath and T.B. Lucatorto, Phys. Rev. Lett. 38, 1390 (1977).
11. R.F. Reilman and S.T. Manson, Astrophys. J. Supp. 40, 815 (1979).
12. W. Ong, S.T. Manson, H.K. Tseng, and R.H. Pratt, Phys. Lett. 69A, 319 (1979).
13. S.T. Manson, J.L. Dehmer, U. Fano, M. Inokuti, and C.E. Theodosiou, IX ICPEAC Abstracts of Papers (U. of Washington Press, Seattle, Washington) 693 (1975).
14. K.D. Chao, J.L. Dehmer, U. Fano, M. Inokuti, S.T. Manson, A. Msezane, R.F. Reilman, and C.E. Theodosiou, in Beam-Foil Spectroscopy, eds. I.A. Sellin and D.J. Pegg (Plenum, N.Y., 1976), p. 637.
15. A.Z. Msezane and S.T. Manson, Phys. Rev. Letters 35, 364 (1975).
16. A.Z. Msezane and S.T. Manson, to be published.
17. D. Ton-That, S.T. Manson, and M.R. Flannery, J.Phys. B 10, 621 (1977).
18. E.W. McDaniel, M.R. Flannery, E.W. Thomas, H.W. Ellis, K.J. McCann, S.T. Manson, J.W. Gallagher, J.R. Rumble, and E.C. Beaty, Compilation of Data Relevant to Nuclear Pumped Lasers, U.S. AMRDC Technical Report H-78-1, Vol. III, IV, and V (1979).
19. S.T. Manson, L.H. Toburen, D.H. Madison, and N. Stolterfoht, Phys. Rev. A 12, 60 (1975).
20. S.T. Manson and L.H. Toburen, IX ICPEAC Abstracts of Papers (U. of Washington Press, Seattle, Washington) 751 (1975).
21. D.H. Madison and S.T. Manson, Phys. Rev. A 20, 825 (1979).
22. L.H. Toburen, S.T. Manson, and Y.-K. Kim, Phys. Rev. A 17, 148 (1978).
23. S.T. Manson, L.H. Toburen, and Y.-K. Kim, X ICPEAC Abstracts of Papers (Comm. a L'Energie Atomique, Paris) 988 (1977).
24. Y.-K. Kim, Radiat. Res. 61, 21 (1975).
25. Y.-K. Kim, Radiat. Res. 64, 205 (1975).
26. S.T. Manson and A. Msezane, J. Phys. B 8, L5 (1975).

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1. "Effects of Minima in the Generalized Oscillator Strength on the Total Ionization Cross Section," S.T. Manson and A. Msezane, Jour. Physics B 8, L5-L7 (1975).

2. "Energy and Angular Distribution of Electrons Ejected from Helium by Fast Protons and Electrons: Theory and Experiment," S.T. Manson, L.H. Toburen, D.H. Madison, and N. Stolterfoht, Physical Review A 12, 60-79 (1975).

3. "New Minima in Photoionization Cross Sections," A.Z. Msezane and S.T. Manson, Physical Review Letters 35, 364-366 (1975).

4. "Dependence of Electron-Scattering Phase Shifts and of Photoabsorption Cross Sections on Both Atomic Number and Ionic Charge for Atomic Ions," S.T. Manson, J.L. Dehmer, U. Fano, M. Inokuti, and C.E. Theodosiou, IX ICPEAC Abstracts of Papers, Univ. of Washington Press, Seattle, Washington, 693-694 (1975).

5. "Energy and Angular Distribution of Electrons Ejected from Ar by 1-MeV Proton Impact Ionization: Theory and Experiment," S.T. Manson and L.H. Toburen, IX ICPEAC Asbtracts of Papers, Univ. of Washington Press, Seattle, Washington, 751-752 (1975).

6. "Photoionization of Positive Ions: The Mercury Isoelectronic Sequence," A.Z. Msezane, and S.T. Manson, IX ICPEAC Abstracts of Papers, Univ. of Washington Press, Seattle, Washington, 1185-1186 (1975).

7. "Relative Intensities in Photoelectron Spectroscopy of Atoms and Molecules," R.F. Reilman, A.Z. Msezane, and S.T. Manson, Jour. Electron Spectroscopy 8, 389-394 (1976).

8. "Satellite Lines in Photoelectron Spectra," S.T. Manson, Jour. Electron Spectroscopy 9, 21-28 (1976).

9. "Spectral and Electron Collision Properties of Atomic Ions," K.D. Chao, J.L. Dehmer, U. Fano, M. Inokuti, S.T. Manson, A. Msezane, R.F. Reilman, and C.E. Theodosiou, in Beam-Foil Spectroscopy, eds. I. A. Sellin and D. Pegg (Plenum Press, N.Y., 1976). pp 637-641.

10. "Atomic Photoelectron Spectroscopy, Part I," Advances in Electronics and Electron Physics 41, 73-111(1976).

11. "Photoionization of Positive Ions: Outer p-Subshells of the Noble-Gas Isoelectronic Sequence," A. Msezane, R.F. Reilman, S.T. Manson, J.R. Swanson, and L. Armstrong, Jr., Physical Review A 15, 668-674 (1977).

12. "Photoionization of Positive Ions. I. Oxygen," D.W. Missavage, S.T. Manson, and C.R. Daum, Physical Review A 15, 1001-1005,(1977).

13. "Further Comments on Atomic Central-Potential Models," S.T. Manson and J.E. Purcell, Physical Review A 15, 1319-1321 (1977).

14. "Energy Distribution of Secondary Electrons Ejected from Krypton by Proton Impact Ionization," S.T. Manson, L.H. Toburen, and Y.-K. Kim, X ICPEAC Abstracts of Papers, Commissariat a L'Energie Atomique, Paris, 988-989 (1977).

15. "Relativistic Calculations of Photoionization Cross Sections of Positive Ions," S.T. Manson and W. Ong, X ICPEAC Abstracts of Papers, Commissariat A L'Energie Atomique, Paris, 1198-1199 (1977).

16. "Atomic Photoelectron Spectroscopy, Part II," Advances in Electronics and Electron Physics 44, 1-32 (1977).

17. "Cross Sections for Excitation and Ionization in e- He($2^{1,3}$S) Collisions," D. Ton-That, S.T. Manson, and M.R. Flannery, J. Phys. B 10, 621-635 (1977).

18. "Energy Distributions of Secondary Electrons. III Projective Energy Dependence for Ionization of He, Ne, and Ar by Protons," L.H. Toburen, S.T. Manson, and Y.-K. Kim, Phys. Rev. A 17, 148-159 (1978).

19. "Photoionization of Positive Ions II. Iron," R.F. Reilman and S.T. Manson, Phys. Rev. A 18, 2124-2130 (1978).

20. "The Calculation of Photoionization Cross Sections: An Atomic View," S.T. Manson in Topics in Applied Physics V. 26: Photoemission in Solids I, eds. M. Cardona and L. Ley (Springer Verlag, Berlin, 1978), pp. 135-163.

21. "Photoabsorption Cross Sections for Positive Ions with $Z \leq 30$," R.F. Reilman and S.T. Manson, Astrophysical Journal Supplement 40, 815-880 (1979).

22. "Doubly Differential Cross Section for Proton-Impact Ionization of Argon," D.H. Madison and S.T. Manson, Phys. Rev. A 20, 825-833 (1979).

23. "Photoionization of Highly Stripped Atomic Ions: Relativistic Calculations," W. Ong, S.T. Manson, H.K. Tseng, and R.H. Pratt, Phys. Letters 69A, 319-321 (1979).

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